

Fidelity between one bipartite quantum state and another undergoing local unitary dynamics

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Abstract

The fidelity and local unitary transformation are two widely useful notions in quantum physics. We study two constrained optimization problems in terms of the maximal and minimal fidelity between two bipartite quantum states undergoing local unitary dynamics. The problems are related to the geometric measure of entanglement and the distillability problem. We show that the problems can be reduced to semi-definite programming optimization problems. We give close-form formulae of the fidelity when the two states are both pure states, or a pure product state and the Werner state. We explain from the point of view of local unitary actions that why the entanglement in Werner states is hard to accessible. For general mixed states, we give upper and lower bounds of the fidelity using tools such as affine fidelity, channels and relative entropy from information theory. We also investigate the power of local unitaries, and the equivalence of the two optimization problems.

Keywords: Fidelity; bipartite state; local unitary transformation; Werner state

1 Introduction

Finding suitable quantities for characterizing the correlations in a bipartite or multipartite quantum state has been an important problem in quantum information theory. Three well-known quantities are entanglement, fidelity and mutual information [1]. Investigating the quantities under unitary dynamics has various physical applications. The local evolution of free entangled states into bound entangled or separable states in finite time presents the phenomenon of sudden death of distillability. In the phenomenon, the fidelity was used to evaluate how close the evolved state is close to the initial state [2]. Next, finding out the local unitary orbits of quantum states characterizes their properties for various quantum-information tasks, and it is also mathematically operational [3]-[8]. By searching for the maximally and minimally

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correlated states on a unitary orbit, the authors in [9] quantified the amount of correlations in terms of the quantum mutual information. The correlations in a multipartite state within the construction of unitary orbits have been also examined [10]. These applications originate from the fact that the unitary dynamics influences the interaction of quantum systems. It is thus a widely concerned question to characterize how heavy the influence can be under certain metric such as the fidelity. The latter has been used to evaluate the entangled photon pairs obtained by experimental heralded generation [11], and the unitary gates of experimentally implementing quantum error correction [12]. In contrast to the global unitary dynamics which involves nonlocal correlation, the local unitary action can be locally performed and does not change the properties of quantum states. Because of the easy accessibility in mathematics, the global unitary dynamics has been studied a lot [13]. In contrast, much less is known about the local unitary dynamics.

In this paper, we study the maximal and minimal fidelity between two bipartite quantum states, one of which undergoes arbitrary local unitary dynamics. To be more specific, let ρ and σ be two bipartite states acting on the Hilbert space $\mathcal{H}_1 \otimes \mathcal{H}_2$ of dimensions $\dim \mathcal{H}_i = d_i$, $i = 1, 2$. Let $U(\mathcal{H}_1)$ be the unitary group on \mathcal{H}_1 . We propose two constrained optimization problems as computing the functionals

$$G_{\max}(\rho, \sigma) := \max_{U_i \in U(\mathcal{H}_i): i=1,2} F(\rho, (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger) \quad (1.1)$$

and

$$G_{\min}(\rho, \sigma) := \min_{U_i \in U(\mathcal{H}_i): i=1,2} F(\rho, (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger) \quad (1.2)$$

where $F(\rho, \sigma) := \text{Tr}(\sqrt{\sqrt{\rho}\sigma\sqrt{\rho}})$ is the fidelity between any two semidefinite positive matrices ρ and σ . Because of the symmetric property of fidelity, the two functionals are unchanged under the exchange of arguments ρ and σ . Note that if the local unitary action is replaced by global unitary action, then the problems have been analytically solved in [13].

Intuitively, the functionals respectively stand for the maximal and minimal distance that local unitary can create between quantum states. The solution to the optimization problems exists because the unitary group is a compact Lie group. We will show that they can indeed be reduced to the well-known semidefinite programming (SDP) problems. So we may efficiently compute the functionals for many states. Then we derive the close-form formulae to the functionals when ρ and σ are both pure states, or a pure product state and the Werner state. We show that in contrast with the separable Werner state, the entangled Werner state of $d > 3$ is closer to the set of pure separable states under local unitary dynamics. In this context, the distillability of two-qubit and two-qutrit Werner states may be distinguished by comparing their G_{\max} . For general mixed states, we derive the upper and lower bounds of the functionals in terms of the monotonicity of fidelity, quantum channel, the affine fidelity, the integral over the unitary group via Haar measure. We also investigate how local unitaries influence the commutativity of quantum states, as well as the equivalence of the two optimization problems.

Our results straightforwardly make progress towards the following quantum-information problems. First, $G_{\max}(\rho, \sigma)$ reduces to the geometric measure of entanglement (GME) when ρ or σ is a pure product state [14, 15]. Mathematically the GME of a quantum state ρ is defined as $\max_{\psi} \langle \psi | \rho | \psi \rangle$ where $|\psi\rangle$ is a product state. It is known that the GME of a bipartite state measures the closest distance between this

state and separable states. It coincides with the intuitive interpretation of the functionals. The GME is a multipartite entanglement measure and has been extensively studied recently [16, 17]. The GME also applies to the construction of initial states for Grover algorithm [19, 18], the discrimination of quantum states under local operations and classical communications (LOCC) [20], and one-way quantum computation [16]. For a review of GME we refer the readers to [17]. Recall that the fully entangled fraction (FEF) for any bipartite state ρ in a $d \otimes d$ system is defined as the maximal overlap with maximally entangled pure states,

$$\max_{U, V \text{ unitaries}} \left\langle \Omega \left| (U \otimes V) \rho (U \otimes V)^\dagger \right| \Omega \right\rangle,$$

where $|\Omega\rangle = \frac{1}{\sqrt{d}} \sum_{j=0}^{d-1} |jj\rangle$ is the maximally entangled state. Then, $G_{\max}(\rho, \sigma)$ is the square root of the FEF when one state of ρ and σ is a maximally entangled state for $d_1 = d_2$ [21]. In this case, the other state of ρ and σ can be any mixed state. The FEF works as the fidelity of optimal teleportation, and thus has experimental significance [22]. The close-form for the FEF in a two-qubit system is derived analytically by using the method of Lagrange multiplier [23]. Second, $G_{\min}(\rho, \sigma)$ is related to the famous distillability problem in entanglement theory. The latter is related to the additivity property of distillable entanglement and the activation of bound entanglement [24]. It is known that a bipartite state ρ is distillable if and only if there exists a positive integer n and a Schmidt-rank two pure state $|\psi\rangle$, such that $\langle \psi | (\rho^{\otimes n})^\Gamma | \psi \rangle < 0$ [25, 26]. Our optimization problems imply that ρ is distillable if and only if $\min_{\lambda \in (0,1)} G_{\min}^2(|\phi_\lambda\rangle, (\rho^{\otimes n})^\Gamma + x\mathbb{1}) < x$, where $|\phi_\lambda\rangle = \sqrt{\lambda}|00\rangle + \sqrt{1-\lambda}|11\rangle$ and x is a positive number such that the second argument is positive semi-definite. We stress that the difficulty of the distillability problem mostly arises from the local unitary orbits involved in the optimization problems above. The distillability problem has turned out to be hard, and a review of recent progress can be found in [27]. All these problems are thus well motivated by the findings in this paper.

The rest of the paper is organized as follows. In Sec. 2, we show that the computation of the two functionals G_{\max} and G_{\min} can be reduced to the SDP problem. Then we derive the close-form formulae of functionals when ρ and σ are both pure states, or a pure product state and the Werner state. We also point out a potential connection between the distillability problem and our optimization problem for G_{\max} . Next, several connections, upper and lower bounds on the functionals are computed in Sec. 3. We discuss in Sec. 4, and conclude in Sec. 5.

2 SDP and analytical formula of functionals

We see that $F(\rho, (U \otimes V)\sigma(U \otimes V)^\dagger)$ is a continuous function over local unitary groups $U(\mathcal{H}_1) \otimes U(\mathcal{H}_2)$. Since $U(\mathcal{H}_1)$ and $U(\mathcal{H}_2)$ are compact Lie groups, it follows that there exists $U_i, V_i \in U(\mathcal{H}_i) (i = 1, 2)$ such that

$$G_{\max}(\rho, \sigma) = F(\rho, (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger) \text{ and } G_{\min}(\rho, \sigma) = F(\rho, (V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger).$$

Denote $\hat{\sigma} := (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger$ and $\tilde{\sigma} := (V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger$. Thus

$$G_{\max}(\rho, \sigma) = F(\rho, \hat{\sigma}) \text{ and } G_{\min}(\rho, \sigma) = F(\rho, \tilde{\sigma}).$$

The SDP has been extensively used to treat the distillability problem [28], the separability problem [29], the quantification of entanglement [30] and so on [31]. The SDP for fidelity between two states is obtained

by Watrous [1]. We show that our problems of computing G_{\max} and G_{\min} can be reduced to the SDP optimization problem [32, 33], as a primal problem below. Let $\tau = \hat{\sigma}$ or $\tilde{\sigma}$. Then

$$\text{maximize:} \quad \frac{1}{2} \left(\text{Tr}(X) + \text{Tr}(X^\dagger) \right), \quad (2.1)$$

$$\text{subject to:} \quad \begin{bmatrix} \rho & X \\ X^\dagger & \tau \end{bmatrix} \geq 0, \quad (2.2)$$

where X is a operator of order $d_1 d_2$. Under the above constraint the optimal value of $\frac{1}{2} (\text{Tr}(X) + \text{Tr}(X^\dagger))$ is fidelity $F(\sigma, \tau)$. Its dual problem is

$$\text{minimize:} \quad \frac{1}{2} (\langle \rho, Y \rangle + \langle \tau, Z \rangle), \quad (2.3)$$

$$\text{subject to:} \quad \begin{bmatrix} Y & -\mathbb{1} \\ -\mathbb{1} & Z \end{bmatrix} \geq 0, \quad (2.4)$$

where Y, Z are Hermitian operators. So we can numerically solve the optimization problems for many states with high efficiency. On the other hand, we can analytically solve the problems for pure states.

Theorem 2.1. *Let $\rho = |\Phi_{12}\rangle\langle\Phi_{12}|$ and $\sigma = |\Psi_{12}\rangle\langle\Psi_{12}|$, where the spectra of reduced density operators ρ_1 and σ_1 are $\{a_1 \geq \dots \geq a_N \geq 0\}$ and $\{b_1 \geq \dots \geq b_N \geq 0\}$, respectively, and $d = d_1 = d_2$. Then $G_{\max}(\rho, \sigma) = \sum_{j=1}^d \sqrt{a_j b_j}$ and $G_{\min}(\rho, \sigma) = 0$.*

Proof. There are two $d_2 \times d_1$ matrices A, B such that $|\Phi_{12}\rangle = \text{vec}(A)$ and $|\Psi_{12}\rangle = \text{vec}(B)$ [1]. Then $(U_1 \otimes U_2)|\Psi_{12}\rangle = \text{vec}(U_1 B U_2^\dagger)$ implies $F(\rho, (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger) = |\text{Tr}(A^\dagger U_1 B U_2^\dagger)|$. Since $\rho_1 = A A^\dagger$ and $\sigma_1 = B B^\dagger$, the first assertion follows from the fact $\max_{U, V} |\text{Tr}(X U Y V)| = \sum_{k=1}^N s_k(X) s_k(Y)$ [34]. The second assertion is equivalent to the fact that the product states in the Schmidt decomposition of $|\Phi_{12}\rangle$ can be by local unitaries converted into states orthogonal to those of $|\Psi_{12}\rangle$. \square

When $|\Phi_{12}\rangle$ is from a maximally entangled basis, the proof for $G_{\min}(\rho, \sigma) = 0$ is similar to the technique for the known quantum super-dense coding. On the other hand, a particular case of this theorem has been used to construct a family of entanglement witnesses [35]. Next if ρ is a pure product state, then $G_{\max}^2(\rho, \sigma)$ amounts to the $S(1)$ -norm $\|\sigma\|_{S(1)}$, which is lower bounded by the $(d_1 + d_2 - 1)$ -th eigenvalue in increasing order of σ [36], where the $S(k)$ -norm of bipartite operator X on $\mathcal{H}_1 \otimes \mathcal{H}_2$ is defined as

$$\|X\|_{S(k)} := \sup_{|u\rangle, |v\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2} \{ |\langle u | X | v \rangle| : \text{SR}(|u\rangle), \text{SR}(|v\rangle) \leq k \}.$$

Here $\text{SR}(|w\rangle)$ stands for the Schmidt-rank of pure bipartite state $|w\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$, i.e. the number of nonvanishing coefficients in Schmidt decomposition of $|w\rangle$.

The problem can be analytically solved for the Werner state $\sigma(t) = \frac{1}{d(d-t)}(\mathbb{1}_d \otimes \mathbb{1}_d - t \sum_{i,j=1}^d |ij\rangle\langle ji|)$, $t \in [-1, 1]$. Indeed [37] implies

$$G_{\max}(\rho, \sigma) = \sqrt{\|\sigma\|_{S(1)}} = \sqrt{\frac{1 + |\min(t, 0)|}{d(d-t)}}. \quad (2.5)$$

One can easily show that the minimum of this functional over t is achievable when $t = 0$. That is, the Werner state becomes the maximally mixed state, which is at the center of the set of separable states.

Next, the maximum of the functional may be reached at two points, $t = -1$ and 1 as plotted in Figure 1. The two points respectively correspond to a separable Werner state and the most entangled Werner state. Figure 1 implies that in contrast with the separable Werner state, the entangled Werner state of $d > 3$ is closer to the set of pure separable states under local unitary dynamics. That is, the entanglement of Werner states might be a more inaccessible quantum correlation than the separability. It is known that two-qubit entangled states are distillable, and it is conjectured that two-qutrit entangled Werner states may be non-distillable [38]. Our inequalities imply that the distillability of Werner states of $d = 2$ and $d > 2$ may be essentially distinguished by their distance to the pure separable states under local unitary dynamics.

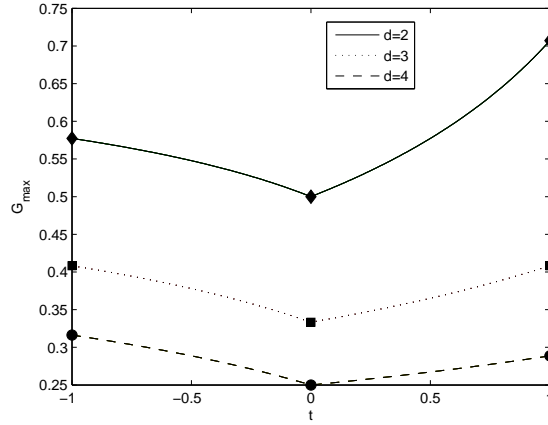


Figure 1: The figure shows the maximum distance between the Werner state and the set of pure product states in terms of the functional G_{\max} . The leftmost value is smaller than the rightmost value for $d = 2$, and bigger than the rightmost value for $d = 4$. The two values are equal for $d = 3$.

In Appendix 5, we also have computed G_{\max} for the pure product state and the isotropic state. In spite of these results, finding the analytical solution to the optimization problems is unlikely because local unitary actions are much more involved than global unitary action U . Indeed, the extremal values of $F(\rho, U\sigma U^\dagger)$ are determined by those global unitary such that the commutator $[\rho, U\sigma U^\dagger] = 0$ [13]. For our purpose we need to replace the global unitary action by local unitary $U_1 \otimes U_2$. We do not know whether there exist U_1 and U_2 such that $F(\rho, (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger)$ can attain its extremal values. In next section we study the upper and lower bounds of G_{\max} and G_{\min} , as well as their connections.

3 Upper and lower bounds of functionals

The optimization problems ask to find out the critical points $\arg G_{\max}(\rho, \sigma)$ and $\arg G_{\min}(\rho, \sigma)$ in the local unitary group, which respectively achieve G_{\max} and G_{\min} . They respectively refer to the local unitary operator $V_1 \otimes V_2$ such that $G_{\max}(\rho, \sigma) = F(\rho, (V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger)$ and $G_{\min}(\rho, \sigma) = F(\rho, (V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger)$. Using these facts, we construct several relations between G_{\max} and G_{\min} . In Proposition 3.1 and

3.2, we show that the sum and difference of G_{\max} and G_{\min} (or their squares) are both upper and lower bounded in terms of some functions of their arguments such as the rank and fidelity. As a result, we study the fidelity inequality in Proposition 3.3, and the affine fidelity of global unitary action in Proposition 3.4. We construct the bounds of G_{\max} and G_{\min} by using the monotonicity of the fidelity, the affine fidelity, the integral over the unitary group via Haar measure, and the relative entropy in Subsect 3.1 and 3.2.

Proposition 3.1. *Let ρ, σ , and $\sigma' = \frac{1}{d_1 d_2 - 1}(\mathbb{1}_{d_1 d_2} - \sigma)$ be three quantum states. We have*

$$\text{rank}(\rho) \geq G_{\max}(\rho, \sigma)^2 + (d_1 d_2 - 1) G_{\min}(\rho, \sigma')^2 \geq 1. \quad (3.1)$$

The first equality holds if there exist two unitary matrices W_1, W_2 such that conditions (i),(ii) and (iii) hold. The second equality holds if and only if there exist two unitary matrices V_1, V_2 such that conditions (iv),(v), and (vi) hold:

- (i) $W_1 \otimes W_2 = \arg G_{\max}(\rho, \sigma) = \arg G_{\min}(\rho, \sigma')$;
- (ii) $\sqrt{\rho}(W_1 \otimes W_2)\sigma(W_1 \otimes W_2)^\dagger \sqrt{\rho}$ and $\sqrt{\rho}(W_1 \otimes W_2)\sigma'(W_1 \otimes W_2)^\dagger \sqrt{\rho}$ both have identical nonzero eigenvalues;
- (iii) $\text{rank}(\sqrt{\rho}(W_1 \otimes W_2)\sqrt{\sigma}) = \text{rank}(\sqrt{\rho}(W_1 \otimes W_2)\sqrt{\sigma'}) = \text{rank}(\rho)$;
- (iv) $V_1 \otimes V_2 = \arg G_{\max}(\rho, \sigma) = \arg G_{\min}(\rho, \sigma')$;
- (v) $\sqrt{\rho}(V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger \sqrt{\rho}$ has rank one;
- (vi) $\sqrt{\rho}(V_1 \otimes V_2)\sigma'(V_1 \otimes V_2)^\dagger \sqrt{\rho}$ has rank one.

The proof is given in Appendix 5. One can easily verify that the second equality in (3.1) holds when ρ is pure, or $\rho = \frac{1}{2}(|00\rangle\langle 00| + |01\rangle\langle 01|)$ and $(V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger = |00\rangle\langle 00|$. In both cases, computing G_{\max} and G_{\min} are equivalent. This is the first connection we have between the two functionals, so it is enough to consider only one of them. We shall discuss the general case in Sec. 4. Furthermore, conditions 5 and 6 imply that ρ has rank at most two. If it has rank two, then conditions 5 and 6 imply that σ is pure. Thus, at least one of ρ and σ is pure when the second equality in (3.1) holds. Next we construct another restriction between G_{\max} and G_{\min} or their squares. This is realized based on the inequalities for the framework of wave-particle duality [39] and the ensembles of Holevo quantity [41].

Proposition 3.2. *Let ρ, σ , and $\sigma' = \frac{1}{d_1 d_2 - 1}(\mathbb{1}_{d_1 d_2} - \sigma)$ be three quantum states. Assume that $U_1 \otimes U_2 = \arg G_{\max}(\rho, \sigma)$ and $V_1 \otimes V_2 = \arg G_{\min}(\rho, \sigma')$. Then*

$$G_{\max}(\rho, \sigma) + G_{\min}(\rho, \sigma') \leq \sqrt{2 + 2F(\hat{\sigma}, \hat{\sigma}')}, \quad (3.2)$$

where $\hat{\sigma} = (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger$ and $\hat{\sigma}' = (V_1 \otimes V_2)\sigma'(V_1 \otimes V_2)^\dagger$. Moreover,

$$\left| G_{\max}^2(\rho, \sigma) - G_{\min}^2(\rho, \sigma') \right| \leq \sqrt{1 - F^2(\hat{\sigma}, \hat{\sigma}')} \quad (3.3)$$

and

$$\left| G_{\max}(\rho, \sigma) - G_{\min}(\rho, \sigma') \right| \leq \sqrt{1 - F^2(\hat{\sigma}, \hat{\sigma}')} \quad (3.4)$$

Proof. The assertion straightforwardly follow from three inequalities in [39, 40] and [41]:

$$\max_{\rho} (F(M, \rho) + F(N, \rho)) = \sqrt{\text{Tr}(M) + \text{Tr}(N) + 2F(M, N)}, \quad (3.5)$$

$$\left| F^2(\sigma, \rho) - F^2(\tau, \rho) \right| \leq \sqrt{1 - F^2(\sigma, \tau)}, \quad (3.6)$$

and

$$|F(\sigma, \rho) - F(\tau, \rho)| \leq \sqrt{1 - F^2(\sigma, \tau)}. \quad (3.7)$$

where M, N are positive semidefinite operators, and ρ, σ, τ are three quantum states. \square

The results show that the characterization of fidelity is important for obtaining a tight bound for the functionals. We study the characterization using an inequality for the approximation of Markov chain property [42].

Proposition 3.3. *Let ρ and σ be two quantum states on \mathbb{C}^d , and Φ be a quantum channel over \mathbb{C}^d . Then*

$$F(\rho, \sigma) \leq \sum_j F(M_j \rho M_j^\dagger, M_j \sigma M_j^\dagger) \leq F(\Phi(\rho), \Phi(\sigma)), \quad (3.8)$$

where $\Phi(*) = \sum_j M_j * M_j^\dagger$ is any Kraus representation of Φ .

Proof. From Lemma B.7 in [42], we know that for an identity resolution $\sum_j E_j = \mathbb{1}$,

$$F(\rho, \sigma) \leq \sum_j F(E_j \rho E_j, \sigma).$$

Since $\Phi(*) = \sum_j M_j * M_j^\dagger$ is a quantum channel, $\sum_k M_j^\dagger M_j = \mathbb{1}$. Assuming $E_j = M_j^\dagger M_j$ in the above inequality, we have

$$F(\rho, \sigma) \leq \sum_j F(M_j^\dagger M_j \rho M_j^\dagger M_j, \sigma). \quad (3.9)$$

Again, by employing the following simple fact, Lemma B.6 in [42], $F(W^\dagger \rho W, \sigma) = F(\rho, W \sigma W^\dagger)$, we obtain the inequality in (3.8). The other inequality is from the concavity of fidelity. \square

Proposition 3.4. *For any given two quantum states ρ and σ on \mathbb{C}^d , there exists a unitary operator U_0 on \mathbb{C}^d , which depends on ρ and σ , such that*

$$F(\rho, \sigma) = A(\rho, U_0 \sigma U_0^\dagger), \quad (3.10)$$

where $A(\rho, \sigma)$ is called affine fidelity [43, 44], defined by $A(\rho, \sigma) := \text{Tr}(\sqrt{\rho} \sqrt{\sigma})$.

Proof. Consider a map defined over the unitary group $U(\mathbb{C}^d)$ in the following:

$$g(U) = A(\rho, U \sigma U^\dagger).$$

Apparently, g is a continuous map over $U(\mathbb{C}^d)$. Furthermore, $g(\mathbb{1}_d) \leq F(\rho, \sigma)$ is a basic matrix inequality. It implies that the affine fidelity is upper bounded by the fidelity. Since the unitary group $U(\mathbb{C}^d)$ is a

compact and connected Lie group, it follows that the image of $U(\mathbb{C}^d)$ under the map g is a closed interval. Thus it suffices to show that there exists a unitary operator V such that $F(\rho, \sigma) \leq g(V)$. We proceed with the following result obtained in [13]: there exists a unitary operator $V \in U(\mathbb{C}^d)$ such that

$$F(\rho, \sigma) = \text{Tr} \left(\exp \left(\log \sqrt{\rho} + V \log \sqrt{\sigma} V^\dagger \right) \right).$$

By Golden-Thompson inequality $\text{Tr} (e^{A+B}) \leq \text{Tr} (e^A e^B)$, where A and B are Hermitian, we get that $F(\rho, \sigma) \leq g(V)$. Now the fidelity $F(\rho, \sigma) \in \text{im}(g)$, the image of g . Therefore there exists a unitary operator $U_0 \in U(\mathbb{C}^d)$ satisfying the property that we want. We are done. \square

In the following two subsections, we will respectively derive the upper and lower bounds of G_{\max} and G_{\min} .

3.1 Bounds of G_{\max}

The monotonicity of the fidelity implies the upper bound

$$G_{\max}(\rho, \sigma) \leq \min \left(\max_{U_1} F(\rho_1, U_1 \sigma_1 U_1^\dagger), \max_{U_2} F(\rho_2, U_2 \sigma_2 U_2^\dagger), \max_{U_{12}} F(\rho, U_{12} \sigma U_{12}^\dagger) \right). \quad (3.11)$$

This bound is analytically derivable, as we have computed explicitly $\max_U F(\rho, U \sigma U^\dagger)$ and $\min_U F(\rho, U \sigma U^\dagger)$ [13]. This result directly applies to the computation of $\max_{U_{12}} F(\rho, U_{12} \sigma U_{12}^\dagger)$. Next we obtain a lower bound of G_{\max} . From a well-known fact in matrix analysis: $|\text{Tr}(A)| \leq \text{Tr}(|A|)$ for any matrix A , where $|A| = \sqrt{A^\dagger A}$, letting $A = \sqrt{\rho} \sqrt{\sigma}$ gives rise to

$$|\text{Tr}(\sqrt{\rho} \sqrt{\sigma})| \leq \text{Tr}(|\sqrt{\rho} \sqrt{\sigma}|).$$

Clearly $\text{Tr}(\sqrt{\rho} \sqrt{\sigma})$ is a nonnegative real number and $F(\rho, \sigma) = \text{Tr}(|\sqrt{\rho} \sqrt{\sigma}|)$, thus $F(\rho, \sigma) \geq A(\rho, \sigma)$ for any two states ρ, σ , then we have

$$\begin{aligned} G_{\max}(\rho, \sigma) &\geq \max_{U_i \in U(\mathcal{H}_i): i=1,2} A(\rho, (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger) \\ &\geq \int_{U(d_1)} \int_{U(d_2)} A(\rho, (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger) d\mu(U_1) d\mu(U_2) \\ &= \frac{\text{Tr}(\sqrt{\rho}) \text{Tr}(\sqrt{\sigma})}{d_1 d_2}. \end{aligned} \quad (3.12)$$

We have denoted the uniform normalized Haar measure by $\mu(U)$ over the unitary group. On the other hand, the inequality [45]

$$S(\rho || \sigma) \geq -2 \log F(\rho, \sigma) \quad (3.13)$$

where $S(\rho || \sigma) := \text{Tr}(\rho(\log \rho - \log \sigma))$ is the quantum relative entropy, implies

$$\min_{U_i \in U(\mathcal{H}_i): i=1,2} S(\rho || (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger) \geq -2 \log G_{\max}(\rho, \sigma). \quad (3.14)$$

So we have obtained a lower bound of (1.1)

$$\begin{aligned} G_{\max}(\rho, \sigma) &\geq \max \left\{ \frac{\text{Tr}(\sqrt{\rho}) \text{Tr}(\sqrt{\sigma})}{d_1 d_2}, \exp \left(-\frac{1}{2} \min_{U_i \in U(\mathcal{H}_i): i=1,2} S(\rho || (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger) \right) \right\}. \end{aligned} \quad (3.15)$$

3.2 Bounds of G_{\min}

Clearly

$$\begin{aligned}
G_{\min}(\rho, \sigma) &\leq \min_{U_2} \int_{U(d_1)} F(\rho, (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger) d\mu(U_1) \\
&\leq \min_{U_2} F(\rho, \mathbb{1}_{d_1}/d_1 \otimes U_2 \sigma U_2^\dagger) \\
&\leq \frac{1}{\sqrt{d_1 d_2}} \text{Tr}(\sqrt{\rho}),
\end{aligned} \tag{3.16}$$

where the last inequality follows from the integral over $U(d_2)$. By exchanging ρ and σ in the inequality, we obtain an upper bound of (1.2)

$$G_{\min}(\rho, \sigma) \leq \frac{1}{\sqrt{d_1 d_2}} \min \{ \text{Tr}(\sqrt{\rho}), \text{Tr}(\sqrt{\sigma}) \}. \tag{3.17}$$

Next, we study the lower bound of G_{\min} . Let $S(\rho) := -\text{Tr}(\rho \log \rho)$ be the von Neumann entropy with the natural logarithm \log and $0 \log 0 \equiv 0$. It is obtained in [46] that for full-ranked states $\rho, \sigma \in D(\mathbb{C}^d)$, we have

$$F(\rho, \sigma) \geq \text{Tr}(\sqrt{\rho}) \times \exp \left(\frac{1}{2} \sum_j \lambda_j^\downarrow(\rho) \log \lambda_j^\uparrow(\sigma) \right), \tag{3.18}$$

where $\lambda^\downarrow(\rho)$ denotes the set of eigenvalues of ρ in the decreasing order and $\lambda^\uparrow(\sigma)$ denotes the set of eigenvalues of σ in the increasing order. It is known that the fidelity is unchanged under the exchange of arguments. Assuming $\rho = \rho, \sigma = (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger$ and exchanging them in (3.18), we obtain a constant lower bound of (1.2)

$$\begin{aligned}
G_{\min}(\rho, \sigma) &\geq \max \left\{ \text{Tr}(\sqrt{\rho}) \times \exp \left(\frac{1}{2} \sum_j \lambda_j^\downarrow(\rho) \log \lambda_j^\uparrow(\sigma) \right), \right. \\
&\quad \text{Tr}(\sqrt{\sigma}) \times \exp \left(\frac{1}{2} \sum_j \lambda_j^\downarrow(\sigma) \log \lambda_j^\uparrow(\rho) \right), \\
&\quad \left. \exp \left(-\frac{1}{2} \max_{U_i \in U(\mathcal{H}_i): i=1,2} S(\rho || (U_1 \otimes U_2) \sigma (U_1 \otimes U_2)^\dagger) \right), \right\}
\end{aligned} \tag{3.19}$$

where the last argument follows from (3.13).

4 Discussion

In this section we investigate the power of local unitaries for the commutativity of quantum states, the quantification of the commutativity, and the equivalence of the two optimization problems. They generalize the previous discussion.

Commutative quantum states can be prepared in the same pure state basis. They not only share operational mathematical properties, and also can save resources in experiments. One might expect that, under local unitary dynamics we could make two non-commutative quantum states become commutative. That is, given two mixed states ρ and σ with $[\rho, \sigma] \neq 0$, are always there local unitaries U_1 and U_2 such

that $[\rho, (U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger] = 0$? Unfortunately The answer is negative. Indeed, let $\rho = \sum_i p_i |a_i\rangle\langle a_i|$ and $\sigma = \sum_j q_j |b_j\rangle\langle b_j|$ be their respective spectral decomposition, and $p_i, q_j > 0$ for all i, j . If the answer is yes, then there exist two sets $\{|a_i\rangle\}$ and $\{|b_j\rangle\}$, such that up to overall phases they are from the same o. n. basis of $\mathcal{H}_1 \otimes \mathcal{H}_2$. Below we construct a counterexample to this statement. Hence the answer is no. We consider two two-qubit states

$$\rho = \frac{1}{2}|\Psi^+\rangle\langle\Psi^+| + \frac{1}{3}|\Psi^-\rangle\langle\Psi^-| + \frac{1}{6}|\Phi^+\rangle\langle\Phi^+|, \quad (4.1)$$

$$\sigma = \frac{2}{3}|00\rangle\langle 00| + \frac{1}{3}|11\rangle\langle 11|, \quad (4.2)$$

where $|\Psi^\pm\rangle = \frac{1}{\sqrt{2}}(|00\rangle \pm |11\rangle)$ and $|\Phi^\pm\rangle = \frac{1}{\sqrt{2}}(|01\rangle \pm |10\rangle)$ are the standard EPR pairs. Since the positive eigenvalues all have multiplicity one, the eigenstates of them of ρ and σ are respectively equal to $\{|\Psi^\pm\rangle, |\Phi^+\rangle\}$ and $\{|00\rangle, |11\rangle\}$, up to overall phases on these states. If the answer is yes, then there are local unitaries U_1, U_2 such that $\{|\Psi^\pm\rangle, |\Phi^+\rangle\}$ and $\{(U_1 \otimes U_2)|00\rangle, (U_1 \otimes U_2)|11\rangle\}$ are from the same o. n. basis of $\mathbb{C}^2 \otimes \mathbb{C}^2$. Since the former consists of entangled states and the latter consists of separable states, they have to be pairwise orthogonal. It is impossible because the former and latter respectively span a 3-dimensional and 2-dimensional subspace in $\mathbb{C}^2 \otimes \mathbb{C}^2$. \square

Another interesting problem is whether the two optimization problems are equivalent for general ρ and σ . The equivalence would imply the sufficiency of solving only one of them. We propose to study two related functionals

$$\max_{U_i \in \mathcal{U}(\mathcal{H}_i): i=1,2} \text{Tr} \left(\rho(U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger \right)$$

and

$$\min_{U_i \in \mathcal{U}(\mathcal{H}_i): i=1,2} \text{Tr} \left(\rho(U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger \right),$$

as they also measure the similarity between mixed states ρ and σ . The computation of the two functionals is equivalent, because if we can compute the former for any ρ and σ , then we can also compute the latter by replacing σ by $\mathbb{1} - \sigma$; and vice versa. So it suffices to compute

$$\max_{U_i \in \mathcal{U}(\mathcal{H}_i): i=1,2} \text{Tr} \left(\rho(U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger \right).$$

Next, it is known that $|\text{Tr}(UA)| \leq \text{Tr}(\sqrt{A^\dagger A})$ for any unitary U and any matrix A . We have

$$\max_{U_i \in \mathcal{U}(\mathcal{H}_i): i=1,2} \text{Tr} \left(\rho(U_1 \otimes U_2)\sigma(U_1 \otimes U_2)^\dagger \right) \leq G_{\max}(\rho^2, \sigma^2). \quad (4.3)$$

So the two functionals are not only physically, but also mathematically related to G_{\max} and G_{\min} .

5 Conclusions

In this paper we have studied two optimization problems that are related to many quantum-information problems. The problems are generally solvable by the SDP, and we managed to work out the analytical formulae for some states. For mixed states we have constructed many upper and lower bounds of the two functionals. We have shown that the entanglement of Werner states might be a more unaccessible quantum correlation than the separability in terms of the local unitary dynamics. We have investigated

the power of local unitaries for the commutativity of quantum states and the equivalence of the two optimization problems. Apart from the problems proposed in last section, studying the relation between the distillability of Werner states and their distance to the separable states may shed new light to the distillability problem.

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Appendix

Isotropic state

The isotropic state is the convex mixture of a maximally entangled state and the maximally mixed state:

$$\rho_{\text{iso}}(\lambda) = \frac{1-\lambda}{d^2-1} (\mathbb{1}_d \otimes \mathbb{1}_d - |\Psi^+\rangle\langle\Psi^+|) + \lambda|\Psi^+\rangle\langle\Psi^+|,$$

where $\lambda \in [0, 1]$ and $|\Psi^+\rangle = \frac{1}{\sqrt{d}} \sum_{j=1}^d |jj\rangle$. By Theorem 2.1, we have

$$\max_{|u\rangle, |v\rangle} |\langle uv|\Psi^+\rangle|^2 = \frac{1}{d} \text{ and } \min_{|u\rangle, |v\rangle} |\langle uv|\Psi^+\rangle|^2 = 0.$$

Thus

$$\langle uv|\rho_{\text{iso}}(\lambda)|uv\rangle = \frac{1-\lambda}{d^2-1} + \frac{d^2\lambda-1}{d^2-1} |\langle uv|\Psi^+\rangle|^2. \quad (5.1)$$

To further characterize the maximum and minimum of this function, we discuss two subcases.

- (1). If $\frac{1}{d^2} \leq \lambda \leq 1$, then $\max_{|u\rangle, |v\rangle} \langle uv|\rho_{\text{iso}}(\lambda)|uv\rangle = \frac{d\lambda+1}{d(d+1)}$ and $\min_{|u\rangle, |v\rangle} \langle uv|\rho_{\text{iso}}(\lambda)|uv\rangle = \frac{1-\lambda}{d^2-1}$;
- (2). If $0 \leq \lambda < \frac{1}{d^2}$, then $\min_{|u\rangle, |v\rangle} \langle uv|\rho_{\text{iso}}(\lambda)|uv\rangle = \frac{d\lambda+1}{d(d+1)}$ and $\max_{|u\rangle, |v\rangle} \langle uv|\rho_{\text{iso}}(\lambda)|uv\rangle = \frac{1-\lambda}{d^2-1}$. In summary, we have

$$G_{\text{max}}(\rho_{\text{iso}}(\lambda), |uv\rangle\langle uv|) = \max \left(\sqrt{\frac{d\lambda+1}{d(d+1)}}, \sqrt{\frac{1-\lambda}{d^2-1}} \right), \quad (5.2)$$

and

$$G_{\text{min}}(\rho_{\text{iso}}(\lambda), |uv\rangle\langle uv|) = \min \left(\sqrt{\frac{d\lambda+1}{d(d+1)}}, \sqrt{\frac{1-\lambda}{d^2-1}} \right). \quad (5.3)$$

Proof of Proposition 3.1

For any semi-definite positive matrix X , the following inequality is easily derived via the spectral decomposition of X :

$$\sqrt{\text{rank}(X) \cdot \text{Tr}(X)} \geq \text{Tr}(\sqrt{X}) \geq \sqrt{\text{Tr}(X)}, \quad (5.4)$$

where the first equality holds if and only if X has identical nonzero eigenvalues, and the second equality holds if and only if X has rank one. Let $X = A^{1/2}BA^{1/2}$ for any two semi-definite positive matrices A, B . Then (5.4) implies

$$\sqrt{\text{rank}(A^{1/2}B^{1/2}) \cdot \text{Tr}(AB)} \geq F(A, B) \geq \sqrt{\text{Tr}(AB)}, \quad (5.5)$$

where the first equality holds if and only if $A^{1/2}BA^{1/2}$ has identical nonzero eigenvalues, and the second equality holds if and only if $A^{1/2}BA^{1/2}$ has rank one. To prove the first inequality in (3.1), let $W_1 \otimes W_2 = \arg G_{\max}(\rho, \sigma)$. We have

$$\begin{aligned} & G_{\max}(\rho, \sigma)^2 + (d_1 d_2 - 1) G_{\min}(\rho, \sigma')^2 \\ & \leq F(\rho, (W_1 \otimes W_2)\sigma(W_1 \otimes W_2)^\dagger)^2 + (d_1 d_2 - 1) F(\rho, (W_1 \otimes W_2)\sigma'(W_1 \otimes W_2)^\dagger)^2 \\ & \leq \text{rank}(\rho^{1/2}(W_1 \otimes W_2)\sigma^{1/2}(W_1 \otimes W_2)^\dagger) \text{Tr} \left(\rho(W_1 \otimes W_2)\sigma(W_1 \otimes W_2)^\dagger \right) \\ & \quad + \text{rank}(\rho^{1/2}(W_1 \otimes W_2)(\sigma')^{1/2}(W_1 \otimes W_2)^\dagger) (d_1 d_2 - 1) \text{Tr} \left(\rho(W_1 \otimes W_2)\sigma'(W_1 \otimes W_2)^\dagger \right) \\ & \leq \text{rank}(\rho) [\text{Tr} \left(\rho(W_1 \otimes W_2)\sigma(W_1 \otimes W_2)^\dagger \right) + (d_1 d_2 - 1) \text{Tr}(\rho(W_1 \otimes W_2)\sigma'(W_1 \otimes W_2)^\dagger)] \\ & = \text{rank}(\rho), \end{aligned} \quad (5.6)$$

where the first inequality follows from the definition of G_{\max} and G_{\min} , and its equality is equivalent to condition (i). The second inequality in (5.6) follows from the first inequality in (5.5) by assuming $A = \rho$, $B = (W_1 \otimes W_2)\sigma(W_1 \otimes W_2)^\dagger$ and $(W_1 \otimes W_2)\sigma'(W_1 \otimes W_2)^\dagger$, respectively. Its equality is equivalent to condition (ii) by the first inequality in (5.5). The third inequality in (5.6) follows from the fact $\text{rank}(A) \geq \text{rank}(A^{1/2}B^{1/2})$. Its equality holds if condition (iii) holds. So we have proved the first inequality, and the three conditions by which the equality holds in (3.1).

To prove the second inequality in (3.1), let $V_1 \otimes V_2 = \arg G_{\min}(\rho, \sigma')$. We have

$$\begin{aligned} & G_{\max}(\rho, \sigma)^2 + (d_1 d_2 - 1) G_{\min}(\rho, \sigma')^2 \\ & \geq F(\rho, (V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger)^2 + (d_1 d_2 - 1) F(\rho, (V_1 \otimes V_2)\sigma'(V_1 \otimes V_2)^\dagger)^2 \\ & \geq \text{Tr}(\rho(V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger) + (d_1 d_2 - 1) \text{Tr}(\rho(V_1 \otimes V_2)\sigma'(V_1 \otimes V_2)^\dagger) \\ & = 1, \end{aligned} \quad (5.7)$$

where the second inequality follows from (5.5) by assuming $A = \rho$, $B = (V_1 \otimes V_2)\sigma(V_1 \otimes V_2)^\dagger$ and $(V_1 \otimes V_2)\sigma'(V_1 \otimes V_2)^\dagger$, respectively. So we have proved the second inequality in (3.1). The equality in (3.1) holds if and only if the first two equalities in (5.7) both hold. The first equality is equivalent to condition (iv) by the definition of G_{\max} and G_{\min} , and the second equality is equivalent to conditions (v) and (vi) by (5.5). This completes the proof.

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